Direct calculation of interfacial tension for lattice models by the Monte Carlo method

K. K. Mon

Department of Physics and Center for Joining of Materials, Carnegie–Mellon University,
Pittsburgh, Pennsylvania 15213

David Jasnow

Department of Physics and Astronomy, University of Pittsburgh,
Pittsburgh, Pennsylvania 15260

(Received 5 March 1984)

We present a novel application of Monte Carlo sampling techniques for the direct evaluation of the interfacial tension that is applicable over a wide range of system sizes and temperatures. The results for the two-dimensional Ising model with system size up to 32×32 for temperature at and below T_c have been analyzed within scaling theory. An accurate estimate for the surface-tension amplitude in excellent agreement with Onsager's exact result is obtained.

Despite extensive current interest in the statistical mechanics of surfaces and interfaces,[1] there has not yet appeared a simple Monte Carlo method for the direct evaluation of interfacial tension that is applicable to large systems and over a range of temperatures. Standard thermodynamic integration techniques are very useful far below the critical temperature (T_c), but become difficult to apply near T_c. Recently, an elegant method based on studies of the order-parameter distribution has been introduced by Binder.[2] The approach appears to be quite successful, but, as was noted,[2] it is limited to temperatures close to T_c and in system size. In this paper we present a novel extension of Monte Carlo sampling techniques for direct evaluation of the interfacial tension, applicable over a wide range of system size and temperature. This method has been applied to the two-dimensional Ising model for system size up to 32×32 and for temperature at and much below T_c. The results have been analyzed within finite-size scaling assumptions and are in excellent agreement with exact results. The approach and results from this initial application are presented here.

A method for evaluation of the surface tension or its analog is also of interest in field-theoretic applications. A class of ferromagnetic Ising models will allow construction of dual models. As noted, for example, by Bricmont, Lebowitz, and Pfister[3] the surface tension of the original Ising model relates to the asymptotic behavior of certain spin correlations in the dual model. For $d = 3$ the dual is the Ising gauge model[4] and the surface tension of the "direct" model equals precisely the coefficient of the area-law decay of the Wilson loop.[4] In $d = 2$ the surface tension equals directly the mass gap or inverse correlation length at the dual temperature.

We consider here a nearest-neighbor ferromagnetic Ising model on a square lattice with $N_y \times N_x$ ($N_y \equiv N$, $N_x = N + 2$) spins ($\sigma_{ij} = \sigma_{x,y} = \pm 1$) with exchange coupling J at temperature T in zero magnetic field. The Ising system is considered under two sets of boundary conditions, as shown schematically in Fig. 1. Periodic boundary conditions are always taken for the top and bottom edges as shown in Figs. 1(a) and 1(b). The boundary conditions $(+ +)$ then refer to the situation shown in Fig. 1(a) in which the first and last columns of spins are *fixed* with value $\sigma = +1$. The alterna-

tive set of boundary conditions $(+ -)$ then refer to the situation of Fig. 1(b). For $T < T_c$ the interfacial tension τ is taken to be[3] the difference of free energies

$$\tau = - k_B T / N \ln \frac{Z_{+-}}{Z_{++}} \quad (\text{as } N \to \infty) \ , \tag{1}$$

where Z_{+-} and Z_{++} are the partition functions for the $N \times (N + 2)$ lattice systems described above. Equation (1) may be rewritten in a form more suitable for Monte Carlo sampling as

$$N\tau_N = - k_B T \ln \langle \exp[- (1/k_B T)(\mathcal{H}_{+-} - \mathcal{H}_{++})] \rangle_{++}$$
$$= - k_B T \ln \langle \exp[- (2J/k_B T)m_s] \rangle_{++} \ , \tag{2}$$
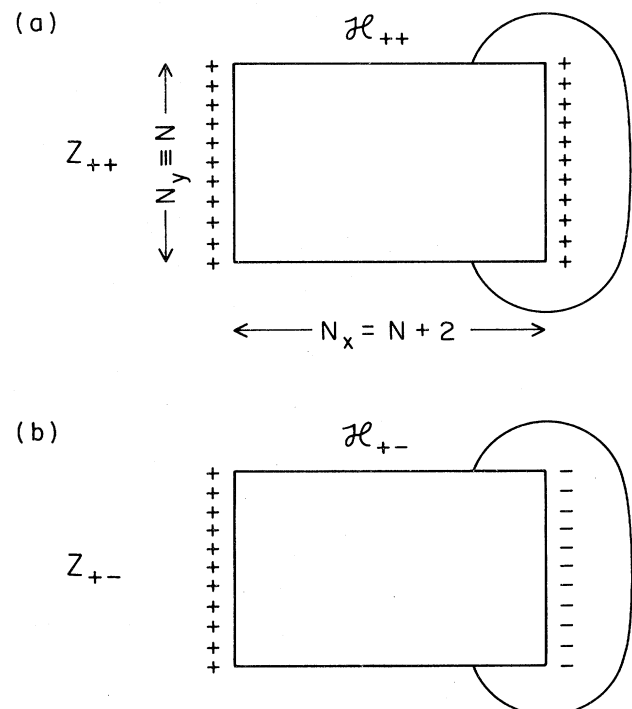

FIG. 1. Boundary conditions for $\mathcal{H}_{++}$ and $\mathcal{H}_{+-}$.

where $m_s = \sum_{i=1}^{N} \sigma_{N+1,i}$ is the magnetization of the layer adjacent to the fixed "all minus" layer shown in Fig. 1(b), and the ensemble average $\langle \ \rangle_{++}$ is generated by the Hamiltonian $\mathscr{H}_{++}$ defined by the $(++)$ boundary condition. The interfacial tension can then be evaluated as an ensemble average.

This formulation represents direct sampling of the difference in free energy between two systems by weighting configurations generated by $(++)$ ensemble. Such a method is useful only when there is sufficient overlap in the configurations sampled by the two ensembles. This then limits its usefulness to very small systems and near T_c.[5] To circumvent this difficulty, observe that Eq. (2) can be rewritten by considering

$$\langle \exp[-(1/k_BT)(\mathscr{H}_{+-} - \mathscr{H}_{++})]\rangle_{++}$$

$$= \frac{\langle \exp[-(1/k_BT)(\mathscr{H}_{+-} - \mathscr{H}')]\rangle_{\mathscr{H}'}}{\langle \exp[-(1/k_BT)(\mathscr{H}_{++} - \mathscr{H}')]\rangle_{\mathscr{H}'}}, \quad (3)$$

where now the ensemble is generated by some Hamiltonian $\mathscr{H}'$ (defined by some boundary conditions) which can be chosen such that overlap of configurations generated by $\mathscr{H}'$ with those of $\mathscr{H}_{+-}$ and $\mathscr{H}_{++}$ is a maximum. Observe that both ensemble averages on the right-hand side of Eq. (3) can be evaluated simultaneously within one single ensemble generated by $\mathscr{H}'$. Although only one stage is used, this formulation is in the spirit of the well-known multistage sampling technique.[6] Its application to the evaluation of the interfacial tension is novel and, as shall be shown below, can be an efficient method for calculating the interfacial tension, even in large systems and well below T_c.

The optimum choice for $\mathscr{H}'$ is found by considering boundary conditions which yield sampling, with comparable frequency, of configurations generated by both $\mathscr{H}_{+-}$ and $\mathscr{H}_{++}$. One such boundary condition which leads to rather efficient sampling is a hybrid boundary condition. The spins on one edge are fixed to be all "+", say, while the spins on the other edge are fixed to be + or − (with numbers $N_+ + N_- = N$) in an *alternating sequence* (see Fig. 2). Although this kind of boundary condition is unbiased with respect to $\mathscr{H}_{+-}$ and $\mathscr{H}_{++}$, configurations with an interface (i.e., those with $\mathscr{H}_{+-}$) occur with probability reduced by $\sim \exp(-\tau N/k_BT)$, where τ is the interfacial tension. This becomes important at low temperature and for large
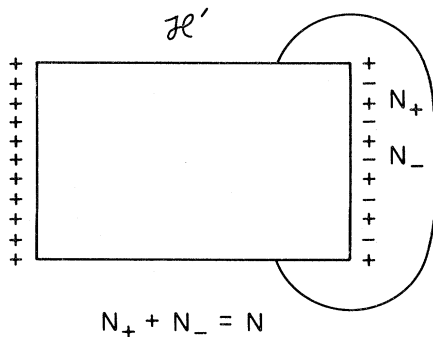
systems, where $\tau N/k_BT$ is large. This difficulty can be reduced in part by choosing on the mixed edge the number of "+" and "−" spins, N_+ and N_-, such that $N_+ < N_-$ which (then) favors sampling more configurations with an interface. We note that the choice of boundary condition (or $\mathscr{H}'$) should only affect the sampling efficiency or the rate of convergence. It does not affect the final results, if sufficiently long sampling is employed to ensure equilibrium. Furthermore, the boundary condition considered here need not be optimum and better choices may exist. However, we have found that for the two-dimensional Ising model, this scheme suffices for size up to $N = 32$ with $\leq 10^6$ Monte Carlo steps per site. This represents the largest system considered in a surface-tension computation.

Our results for the interfacial tension of the two-dimensional Ising models is given in Fig. 3. A few low-temperature cases have been considered for the purpose of illustrating that the method works well in that region. Note that there is excellent overall agreement with Onsager's exact result.[7] By considering a system size N from 2 to 32, for temperatures near and at T_c, we have been able to use the finite-size scaling behavior of the interfacial tension. In analogy with the usual assumptions,[8] we make a scaling ansatz:

$$\tau = \tau_0 t^\mu \sum(x)$$

with

$$x = c_L N^{1/\nu} t, \quad t = \frac{T_c - T}{T_c}. \quad (4)$$

Here μ and ν are the appropriate critical indices for the interfacial tension and correlation length, respectively, and τ_0 and c_L are nonuniversal constants. The universal scaling function $\sum(x)$ has the asymptotic limits, $\sum(x = \infty) = 1$ and $\sum(x \to 0) \sim x^{-\mu}$. For the two-dimensional Ising model, $\mu = \nu = 1$. The limiting forms of $\sum(x)$ are such that $\tau \sim t^\mu$ in the thermodynamic limit, and that *at* the bulk critical temperature, $\tau \sim N^{-\mu/\nu} \sim N^{-1}$. The critical temperature $J/k_BT_c = 0.440\,68 \ldots$ is, of course, known exactly; accordingly, a plot of τN vs N at T_c is made in Fig. 4. The asymptotic limit appears to be reached for $N \geq 8$, the results being consistent with $\tau \sim N^{-1}$.

It is of considerable interest to evaluate as precisely as possible a universal ratio involving the surface-tension am-

FIG. 2. Boundary conditions for $\mathscr{H}'$ of Eq. (3). N_+ is the number of sites fixed in the + configuration and N_- is the number of sites fixed in the − configuration. Note that N_+ need not equal N_-.
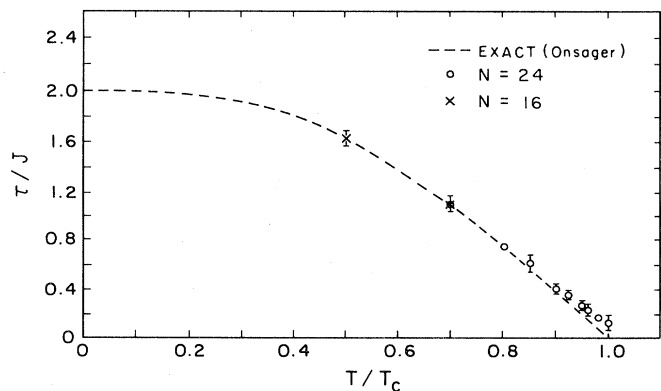

FIG. 3. Comparison of representative Monte Carlo results with exact solution for the infinite system by Onsager (Ref. 6).
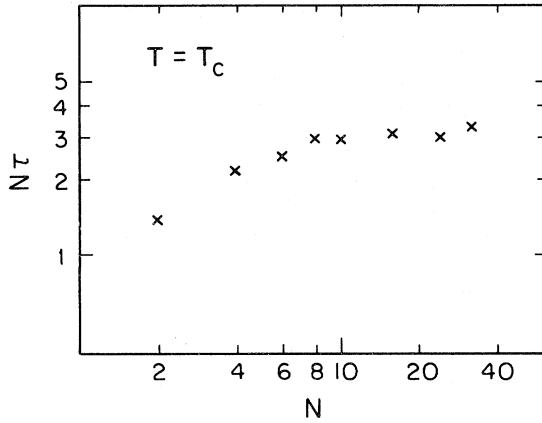
FIG. 4. Finite-size scaling analysis for $T = T_c$ or $t = 0$, for $N = 2$ to 32. Results for $N = 2$ and 4 are exact.

FIG. 5. Finite-size scaling analysis for $T < T_c$ with $N \lesssim 32$. The ratio τ/t^μ approaches τ_0 in the limit of large x ($N^{\mu/\nu}t^\mu$). The exact result (Ref. 7) is indicated and the solid line is an extrapolation of data at $t = 0.01$ using Eq. (10). The dash-dot line indicates some deviations when using data far from T_c ($t \lesssim 0.20$).

plitude τ_0. Such information is needed, for example, in discussions of critical wetting.[9] The simplest relation involves the specific heat, which may be written analogously to (4) as

$$C = \frac{A_0}{\alpha} t^{-\alpha} W(x) \quad , \tag{5}$$

with $W(x) \to 1$ as $x \to \infty$ (thermodynamic limit) and as usual $W(x) \to x^\alpha$ as $x \to 0$. The ratio is, in the thermodynamic limit, given by[10]

$$U_\tau = \lim_{\tau \to 0} \frac{\tau(t)/k_B T_c}{[\alpha t^2 C(t)]^{(d-1)/d}}$$

$$= \frac{\tau_0/k_B T_c}{A_0^{(d-1)/d}} \quad . \tag{6}$$

Unfortunately, a finite-size extrapolation *at* $T = T_c$ is not sufficient to extract U_τ because subdominant parts of the scaling functions as $x \to 0$ are required but cannot be determined with the size systems one may realistically treat.

By probing away from but near $T = T_c$ one may plot $\tau t^{-\mu}$ vs $N^{1/\nu}t$. One must reach the scaling limit; according to Eq. (4) the asymptotic value for large $N^{1/\nu}t$ yields τ_0. This plot is shown for the $d = 2$ Ising model in Fig. 5. For size 32×32 (with $t = 0.05$) the value is still about 20% above the exact value. Nonetheless, this represents considerable progress, and larger systems can in principle be considered within this approach. Also shown in Fig. 5 are points corresponding to $t = 0.1$ and 0.2. The danger of trying to reach the scaling limit (large $tN^{1/\nu}$) by taking too-large values of t is clearly demonstrated. The amplitude A_0 is exactly known in $d = 2$, but more generally it would have to be determined from a finite-size analysis as well (off T_c).

Further progress can be made without using excessively large system by considering alternative means of analysis. This is motivated by the following observations. The difficulty with $\Sigma(x)$ is related to its slow approach toward the large x limit of $\Sigma(\infty) = 1$. One may surmise that this is related to the $x \to 0$ limits where $\Sigma(x \to 0) \cong Bx^{-\mu}$ diverges. This limiting property incorporates the scaling of the surface tension at $t = 0$ which is, $\tau_N(t = 0) \cong \tau_0 B c_L^{-\mu} N^{-\mu/\nu}$. Here, c_L is a nonuniversal amplitude related to the correlation length and B is a universal constant. We will consider removing this singular part from $\Sigma(x)$ by adding and subtracting $Bx^{-\mu}$ and introducing $Y(x)$ with $\Sigma(x) = Bx^{-\mu}$
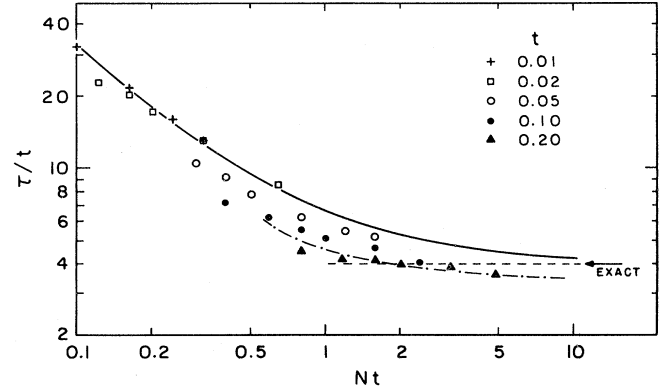
$+ Y(x)$. The surface-tension expression Eq. (4) becomes

$$\tau_N(t) = \tau_N(t = 0) + \tau_0 t^\mu Y(x) \quad . \tag{7}$$

The limiting forms are $Y(x) \to 1$ as $x \to \infty$, and as $x \to 0$ with $t \to 0$, $t^\mu Y(x) \to 0$. It is sufficient to assume

$$Y(x \to 0) \cong B' x^{-\mu'} \text{ as } x \to 0 \quad , \tag{8}$$

with $0 \leqslant \mu' < \mu$ and B' is an additional amplitude, which merely asserts a power law for the subdominant part of the original $\Sigma(x)$. This then suggests considering

$$N^{\mu/\nu}\tau_N(t) = N^{\mu/\nu}\tau_N(t = 0) + N^{\mu/\nu}t^\mu \tau_0 Y(x) \tag{9}$$

and a plot of $N^{\mu/\nu}\tau_N(t)$ vs $N^{\mu/\nu}t^\mu$ to obtain τ_0 as the limiting slope with large x. $N^{\mu/\nu}\tau_N(t = 0)$ would also be obtained as the intercept by extrapolating back to $x = 0$. With this analysis for the data at $t = 0.01$, we found that for $N \geqslant 16(N^{\mu/\nu}t^\nu \geqslant 0.16)$, $Y(x)$ has reached its large-x limit. We obtain $\tau_0 = 3.96 \pm 0.2$ and $N^{\mu/\nu}\tau_N(t = 0) = 2.9 \pm 0.2$. The exact result of Onsager[7] is $\tau_0 = 3.99 \ldots$, and the estimate for $N^{\mu/\nu}\tau_N(t = 0)$ from scaling analysis of the data at $t = 0$ is 3.0 ± 0.3. (See Fig. 4.) An "approximant" for $N^{\mu/\nu}t^\mu \geq 0.16$ is then suggested,

$$\Sigma(x) \cong 1 + Bx^{-\mu}$$

$$= 1 + 0.7323(N^{1/\nu}t)^{-\mu} \quad , \tag{10}$$

which is shown as the solid curve in Fig. 5.

Observe that Eq. (10) has the correct large and small x limits. These suggested results are obtained in the finite-size region and may shed some light on the structure of the scaling function in that region. Such information may prove useful for simulations of Ising and other systems.

We have described a method for direct evaluation of interfacial tension which is applicable to large systems at or below T_c. Although for the system sizes and temperatures considered the one-stage formulation suffices, for much larger systems ($N \gg 32$) and lower temperatures, multistage extension of Eq. (3) would be necessary, but is straightforward. The important observation is that computational efforts (or number of stages) would only increase roughly linearly with system size or on lowering tempera-

ture. Thus, this method should be a useful technique in the study of interfaces for large systems and in three dimensions where a considerable number of important problems await solution. Preliminary work on the $d = 3$ case is encouraging.

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